EXERCISES

Computational Materials Science

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SHEET 1

Exercise 1: Density functional theory

Goal of this exercise: Use the WIEN2k code to calculate (1) the ground state energy, (2) partial densities of states (DOS) and (3) the bandstructure of $SrVO_3$. Below is a list of steps to guide you, see the user guide available at http://www.wien2k.at/reg_user/textbooks for details. Answers to the questions included below (including plots) should be sent by email to *both* held@ifp.tuwien.ac.at and assmann@ifp.tuwien.ac.at.

Strontium vanadate $SrVO_3$ is a *cubic perovskite* (space group 221, $Pm\bar{3}m$) with a lattice constant of 3.8425 Å and atoms at the positions
Sr (0, 0, 0), V (½, ½, ½), O (0, ½, ½), O (½, 0, ½), O (½, ½, 0)

0. In a terminal, run the command `w2web` to start the *wien2web* server. Open the URL that it prints in a web browser.

1. Create a session for $SrVO_3$ and start *StructGen* to create the "master input file" `SrVO3.struct`. Follow the instructions to set the *muffin-tin radii* (RMT) and save the structure; view it with XCrysDen to make sure it is correct.

Q1. Save a picture of your crystal structure.

2. Choose *initialize calculation* and follow the steps. In this case you can use the defaults, but try to understand the output you will see.

Q2. After the initialization (specifically, after `symmetry`), the `struct` file is now complete. Read it: How many atoms are there? How many symmetry operations? Consider symmetry operations nos. 48 and 29, and explain what they mean.

Q3. `kgen` generated a list of *k-points* to span the Brillouin zone. How many k-points did you request in the initialization? How many are there in the `klist` file?

3. You are now ready for your first DFT calculation *(run SCF)*.

Q4. While the calculation is running, monitor its progress *(Utils / analysis)*. Save a plot of the convergence of energy and charge-distance. When the calculation is done, you are in a position to give the answer for our first goal above: What is the ground state energy of $SrVO_3$?*

*But note that this number by itself means very little as it depends on the details of the calculation. Only a comparison of energies (e.g. with different atomic positions) is really meaningful.

4. Calculate and plot the density of states *(Tasks / DOS)*. Calculate at least the total DOS and the V-t_{2g} and V-e_g contributions.

Q5. The DOS contains a lot of "physics" in a concise manner. Which are the most "important" contributions? Compare the t_{2g} and e_g contributions of V. Which one is higher in energy? Can you say why? You can also identify DOS which states hybridize with each other ($\rightsquigarrow$ bonding in the crystal).

5. Calculate and plot the bandstructure *(Tasks / Bandstructure)*.

Q6. How are DOS and bandstructure related—which one could be derived (in principle) from which, and how? Can you identify some of the bands (which atoms/states they correspond to)?

6. You are now done with the compulsory part of the exercise—time to have some fun! Here are some suggestions, approximately in increasing order of difficulty:

- Check to see if the various "quality settings" of the calculation (number of k-points, $RK_{\max}$, ...) we used are good enough. (How would you check that? How do you define "good enough"?)
- Make a *band character* (or "fat bands") plot. Which band character would you choose?
- Try a different functional. Which one did you use up to now? Which other functionals do you know? What is the role of the "functional" in this context?
- Plot the optical conductivity. Identify different contributions (hint: compare to the DOS).
- Plot the electron density. There are many options: 2d/3d, SCF density/difference density, valence density/total density, ...– What do "density/difference" and "valence/total" mean?